

1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-  
59950-41-3 | DTXSID40208664

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 9.04

Global applicability domain: Inside

Local applicability domain index: 9.71e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>3,3',4,4'-Tetrachlorobinphenyl</div> <div>Measured: 9.70</div> <div>Predicted: 8.88</div>	<div>Image not found</div> <div>2,3,4,5-Tetrachlorobiphenyl</div> <div>Measured: 8.74</div> <div>Predicted: 8.87</div>	<div>Image not found</div> <div>Pyrene</div> <div>Measured: 8.80</div> <div>Predicted: 8.87</div>
<div>Image not found</div> <div>Fluoranthene</div> <div>Measured: 8.88</div> <div>Predicted: 8.87</div>	<div>Image not found</div> <div>2,3',4,4'-Tetrachlorobiphenyl</div> <div>Measured: 9.02</div> <div>Predicted: 8.77</div>	